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The elegance of disordered granular packings: a validation of Edwards' hypothesis

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We have found a way to analyze Edwards' density of states for static granular packings in the special case of round, rigid, frictionless grains assuming constant coordination number. It obtains the most entropic density of single grain states, which predicts several observables including the distribution of contact forces. We compare these results against empirical data obtained in dynamic simulations of granular packings. The agreement between theory and the empirics is quite good, helping validate the use of statistical mechanics methods in granular physics. The differences between theory and empirics are mainly due to the variable coordination number, and when the empirical data are sorted by that number we obtain several insights that suggest an underlying elegance in the density of states.

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The intriguing behaviors of sand and other granular materials are not well understood from a fundamental point of view [1] and there is no theory with a pedigree equivalent to the Navier-Stokes or Maxwell's equations to explain how their state evolves over time, even in the most commonly occurring scenarios. Considering the ubiquity of granular materials in nature, this is quite surprising. Making a new effort to explain their physics, Edwards, *et al.*, have proposed that the methods of statistical mechanics may be successfully applied [2]. They hypothesized *a priori* a flat measure in the statistical ensemble—that every metastable arrangement of grains (a *blocked* state) is equally probable under certain conditions—and that the analysis of this ensemble should predict some of the important behaviors.

There is no theoretical proof of ergodicity for granular materials, and so it is an important question whether or not the nonlinear, lossy dynamics of granular materials might produce significant selection effects, biasing the measure so that Edwards' hypothesis would not be correct. Seeking to answer this, a number of empirical tests have been performed by computer simulation. In these, Edwards' hypothesis has successfully predicted packing behaviors for several idealized models [3] and the diffusion-mobility behavior of individual grains when a simulated packing is slowly sheared [4]. In both cases it appears that the dynamics cause the geometry of the model to explore some region of the phase space with sufficient ergodicity to justify the flat measure.

In this Letter we present a different kind of test for Edwards' hypothesis. Rather than examining the geometric features of the packing, we demonstrate that Edwards' flat measure correctly predicts the distributions for single grain load states and for contact forces. This prediction is centrally important to a statistical mechanics

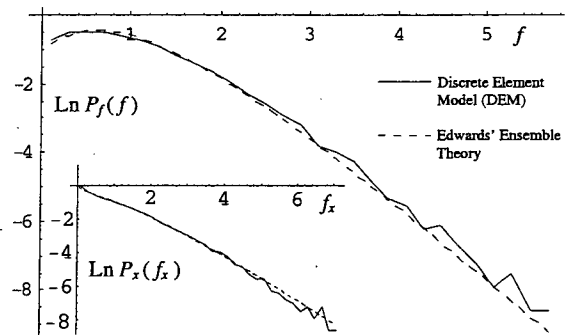


FIG. 1: (Semilogarithmic) Distribution of granular contact force magnitudes $P_f(f)$ (main graph) and Cartesian components $P_x(f_x)$ (inset). The theory and the empirical discrete element model (DEM) data are strikingly in agreement. Because the form of $P_f(f)$ reflects the important organizational features of quasi-static granular physics, this result implies that Edwards' hypothesis is sufficient to capture that physics.

theory because a distribution reflects how the ensemble is organized and demonstrates whether or not the correct physics have been incorporated. In particular, Edwards' hypothesis should predict at least three features in the contact force distribution $P_f(f)$ as illustrated in Fig. 1: the wide tail [5] related to the heterogeneity of stresses in a packing (*force chains*) [6]; the small peak near the average value of force under isotropic conditions [7] related to static equilibrium of the grains (*jamming*) [8]; and the non-zero probability density at zero force, $P_f(0) > 0$, related to the tipping of grains (*fragility*) [9]. The combination of these three features is unique to the granular distribution, not being found in the typical densities of states for thermal systems. If Edwards' hypothesis fails

to produce this form then it is doubtful that it could become the basis for a theory of quasi-static rheology, since the tipping or sliding of individual grains depends upon the state of their contact forces.

This Letter will address the question first by analyzing the density of states (DOS) from first principles, which results in a transport equation. We will present the distributions that are the numerical solution to the transport equation. We have performed Discrete Element Modeling (DEM) [10] for granular packings under conditions similar to those assumed by the theory. The comparison of the two supports the sufficiency of Edwards' hypothesis and provides new insight into the form of the DOS.

Following Edwards and coworkers [11], we focus on the case of amorphous packings of cohesionless, rigid grains all having the same coordination number Z that makes the packing isostatic [12]. Our case is further idealized by using two dimensional round grains with monodisperse grain diameters, omitting gravity and working in the thermodynamic limit (infinitely large packings) so that the boundary layer may be neglected. We focus on the frictionless case so that $Z = 4$, and we limit this Letter to isotropic stress and fabric although the transport equation can solve for anisotropic cases, too. The idealizations may be taken out in future refinements of the theory, but this is a good starting point because packings of cohesionless, round grains that are perfectly rigid [13] and/or frictionless [14, 15] and/or monodisperse [7, 15] have been the focus of many empirical studies and are known to have force distributions with the same features as the less idealized packings. Hence they must be subject to the same basic organization in the physics.

Our avoidance of friction is especially important because it is known that 2D round, rigid, frictionless packings in dynamic simulations actually do have an average coordination $\langle Z \rangle = 4$ such that they are isostatic, whereas frictional packings are hyperstatic. Isostaticity means that a blocked state subjected to a particular stress condition will correspond to only one microstate of contact forces between the grains. Hyperstatic ensembles have been recently analyzed [16], in which each blocked state corresponds to more than one microstate of contact forces—a “solution space” with non-zero volume. It has been shown that common dynamic modeling techniques do not sample that solution space uniformly [17], so it would be difficult to compare the forces predicted by Edwards' hypothesis with those resulting from dynamic modeling in a hyperstatic case. While the issues surrounding hyperstaticity are clearly important, we avoid them here so that we may test Edwards' hypothesis.

The goal of the analysis is to combine Edwards' micro-canonical DOS [18] and contact force probability functional [11] and derive the density of single grain states

$\rho_g(w_x, w_y, \theta_1, \dots, \theta_4)$. The *Cartesian loads* are

$$w_x = \frac{1}{2} \sum_{\gamma=1}^4 f_{\gamma} |\cos \theta_{\gamma}|, \quad w_y = \frac{1}{2} \sum_{\gamma=1}^4 f_{\gamma} |\sin \theta_{\gamma}|. \quad (1)$$

where f_{γ} and θ_{γ} are the four contact forces and contact angles on a grain. In the special case we have selected, solving for ρ_g provides everything that can be known about the individual grains in the packing. For example, it contains the joint distribution of contact forces and angles,

$$P_{f\theta}(f, \theta) = \int_0^{\infty} d^2 w \int_0^{2\pi} d^4 \theta \rho_g \times \frac{1}{4} \sum_{\gamma=1}^4 \delta(\theta - \theta_{\gamma}) \times \delta[f - f_{\gamma}(w_x, w_y, \theta_1, \dots, \theta_4)], \quad (2)$$

and the generalized fabric distribution $P_{4\theta}(\theta_1, \dots, \theta_4)$ [19].

The analytical method is to count states in Edwards' ensemble and maximize entropy applying the same well-known procedure that has been used to derive the Bose or Fermi energy distributions [20]. Several innovations were needed to apply this procedure to static granular packings as discussed in [21]. The result is

$$\rho_g(w_x, w_y, \theta_1, \dots, \theta_4) = G(\theta_1, \dots, \theta_4) e^{-\lambda_x w_x - \lambda_y w_y} \times \prod_{\gamma=1}^4 [P_{f\theta}(f_{\gamma}, \theta_{\gamma})]^{1/2} \Theta(f_{\gamma}), \quad (3)$$

where Θ is the Heaviside (unit step) function, λ_x and λ_y are the Lagrange multipliers that scale mechanical loading, and G is the Fabric Partition Factor that derives from the array of Lagrange multipliers used to conserve $P_{4\theta}$. Eqs. (2) and (3) form a recursion in $P_{f\theta}$ and ρ_g , the “transport” equation, which may be solved numerically using $P_{4\theta}$ and the mechanical loading as inputs. For the present this has been solved for the isotropic case using the Mean Structure Approximation (MSA), the details of which are in Ref. [21].

To compare with the theory, we have performed DEM simulations of 17,000 two dimensional, round, frictionless grains. A portion of a packing is shown in Fig. 2 to contrast the spatial disorder of the force network with the simplicity of the statistics, discussed below. The grain diameters were uniformly distributed from 1.0 to 1.5 to reduce crystallization. The grains were deposited isotropically into a square test cell with hard walls and without gravity, and their diameters increased by rescaling, producing the desired isotropic stress state. The grains were allowed to move dynamically until they located and settled into a blocked state. They have a linear spring contact law, but staying near the jamming transition avoids excessive deformation of the contacts and approximates the grain rigidity of the analysis. Data from grains in the boundary layer (chosen to be 4 grain

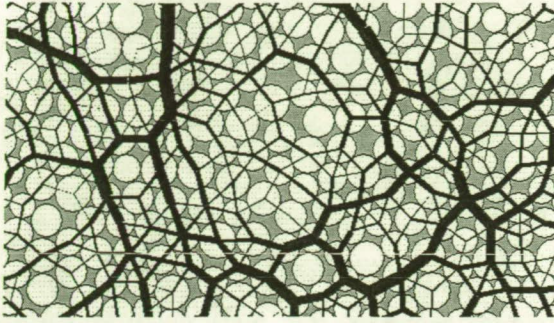


FIG. 2: Portion of a Discrete Element Model (DEM) showing the disordered packing fabric and propagation of force chains. Although disordered, a simple pattern can be discerned in the distribution of load anisotropies, s , and total loads, t . These functional forms of these distributions, as well as $P_f(f)$ and $P_x(f_x)$, are correctly predicted by the transport equation based on Edwards' hypothesis.

diameters along each wall) were discarded to reduce the boundary effects, which we found will otherwise significantly skew the statistics.

Fig. 1 shows the DEM results compared to the theory for $P_f(f)$ and for the distribution of Cartesian components of force, $P_x(f_x)$. The two inflections in $P_x(f_x)$ are characteristic of modified Bessel functions of the second kind, and so we see that the theory successfully predicts the functional form. In the isotropic case $P_f(f)$ can be analytically derived from $P_x(f_x)$, and so its functional form must be an exponential with a polynomial prefactor [21, 22]. It appears there is some error in the region of weak forces (better seen on a linear plot), mostly attributable to the theory's constant $Z = 4$ for every grain as further discussed below. In the DEM there are significant populations for $Z = 3, 4$, and 5.

To convey the other ρ_g information from this solution we might note that w_x and w_y are not statistically independent and therefore plot their statistics as a joint distribution. However, the mean structure theory predicts that the change of variables to *total load*, $t = w_x + w_y$, and *load anisotropy*, $s = (w_x - w_y)/t$, achieves (approximate) statistical independence so that they can be separated more meaningfully. The distribution of load anisotropy, $P_s(s)$, is shown in Fig. 3, demonstrating remarkable agreement between DEM and theory. We can fit a functional form to both, $P_s(s) = \cos(\pi s/2) \exp(-8s^2)$. The cosine arises in the transport equation due to the structural connectedness of the packing, and the Gaussian factor due to a grain's stability space. We segregated the DEM's grains into populations with $Z = 3, 4$, or 5 and plotted $P_s(s)$ for each in Fig. 4. A reasonably good fit to all populations is made simply by writing the Gaussian's standard deviation as $\sigma = 1/Z$. However, the fit is not perfect. The structural connectedness of a grain implies that a Z -dependency should exist in the cosine factor.

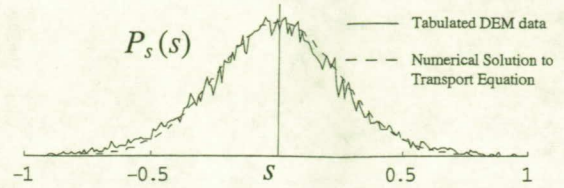


FIG. 3: Distribution of load anisotropy s depicting single grain states. Solid curve—DEM. Dashed curve—theoretical prediction, the numerical solution of the transport equation. The excellent fit helps validate the theory.

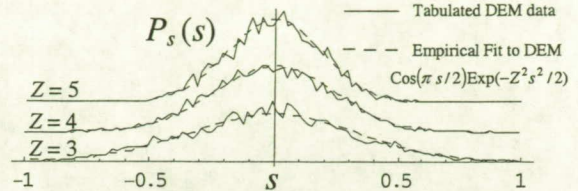


FIG. 4: The same load anisotropy distribution from the DEM as in Fig. 3 except segregated into three graphs by grain coordination number Z (shifted vertically for clarity). An empirical fit was suggested by the theory (dashed curves) which fits all three Z populations when the standard deviation $\sigma = 1/Z$ is the only parameter. Despite the disorder of a granular packing, this result hints at an underlying elegance in the DOS.

We found from the DEM data that the distribution of normalized total loads, $P_t(t)$, is very sensitive to Z and does not compare well with the theory in the region $t < 1$. Segregating by Z populations as shown in Fig. 5, we see that the error in the region $t < 1$ is primarily due to the $Z = 3$ population, the other populations being reasonably well predicted the theory in that region. Knowing that the theory's numerical solution is fitted by the functional form $P_t(t) = t^\alpha e^{-\beta t}$, we tried the same form for all three Z populations, too. We find that all three are described excellently by $\beta = 2Z - 4$ and $\alpha = \beta - 1$. This can be written neatly by defining a convolution operator \mathbb{C}^m such that $\mathbb{C}^m[f(t)]$ convolves m functions $f(t)$ together. Then $P_t(t) = \mathbb{C}^m[e^{-t}]$ where $m = 2Z - 4$ for all Z . This unifying expression along with the beauty of Fig. 5 speaks that this is not an empirical coincidence. It strongly implies the existence of a basis change in the phase space such that the packing's contact forces are resolved into the *loading modes* of the grains, modes which are statistically independent at the grain (hence the convolutions) and canonical (hence the Gibbs distributions e^{-t}). The number of a grain's loading modes m is not generally the number of its contacts Z , so the information contained in the new bases is not localized in the fabric. However, $\langle m \rangle = \langle Z \rangle$ exactly, so the change in basis preserves the overall dimensionality of the space. This forms an interesting analogy to the

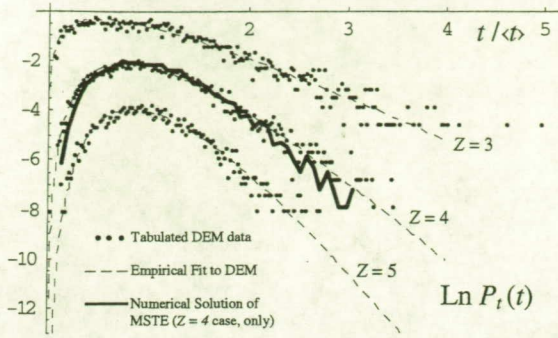


FIG. 5: Distribution of total load t depicting single grain states in the DEM, segregated into three graphs by their coordination number Z (shifted vertically for clarity). The theory does not address the differences between Z populations, but it does imply a particular functional form. The empirical fits based on that form are $P_t(t) = t^{(2Z-5)}e^{-(2Z-4)t}$. As discussed in the text, this implies an elegant result that has far-reaching implications.

molecular vibrations in a solid, which are resolvable into non-localized phonons. While we are accustomed to finding such elegant results in ergodic thermal systems, we did not expect to find the elegance of canonical statistics lying hidden within the untidiness of a granular packing.

In summary, it is clear that the transport equation needs to be generalized beyond the constant $Z = 4$ approximation, but nevertheless its quantitative predictions for $P_f(f)$, $P_x(f_x)$, and $P_s(s)$ are quite good. The prediction of $P_t(t)$ is good, too, when restricted to the relevant $Z = 4$ case. By finding functional fits to the theory we discover simple generalizations that describe each of the Z populations distinctly, demonstrating simplicity in the statistics. An unintended benefit is that this pointed toward a previously unrecognized canonical picture in the t distributions. These are all outstanding confirmations of the theory. Returning to the original goal of this Letter, we conclude that the $P_f(f)$ seen in a dynamic simulation is not indicating any dynamical bias in the measure, but only the features that Edwards' hypothesis predicts. Therefore, the important granular phenomena that are known to produce those features, such as the formation of force chains and the diminishing number of very weak forces after the jamming transition, are also contained as inherent elements of Edwards' ensemble without recourse to the individual grains' dynamics. Since it is the state of these contact forces that determines which grains tip and roll during quasi-static rheology, this implies that Edwards' hypothesis may eventually prove sufficient for the development of a first-principles rheological theory.

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